Exact Ground States and Excited States of Net Spin Models

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Abstract

We study a set of exactly soluble net spin models. There exist two kinds of ground state, one is a complete dimerized state, and the other one is the ground state of corresponding spin-1 model. For the excitation gap, various phases were discovered and determined.

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It is well known that a spin-1/2 antiferromagnetic chain with nearest-neighbor coupling J_1 and next neighbor coupling J_2 could dimerize in the presence of frustration, as exemplified by the exactly soluble one-dimensional Majumdar-Ghosh model [1], where the exact (twofold degenerate) ground state is a simple product of singlet dimers. The elementary excitation can be constructed as a pair of unbound spins above the completely dimerized state [2]. This model also can be considered as a two-chain with one diagonal or a zigzag spin ladder. Analytical and numerical studies [3–5] of the model show a transition from a gapless phase when $J_2 < J_{2c}$ to a gapped phase when $J_2 > J_{2c}$. Recently, the Majumdar-Ghosh model was studied by the density matrix renormalization group (DMRG) approach. The DMRG study of Chitra et al. [6] considered a more general model which included a dimerization term. White and Affleck [7] studied the zigzag spin ladder by using the bosonization and the DMRG methods. In particular, they pointed out a potential important connection between the zigzag chain and the generalized Kondo lattice. In addition, a family of spin-ladder models were studied by Kolezhuk and Mikeska [8] that exhibit non-Haldane spin-liquid properties as predicted by Nersesyan and Tsvelik [9].

In this Letter we consider a set of spin-1/2 antiferromagnetic Heisenberg models defined on a double layer as shown in Fig. 1. Each layer has $M \times L$ sites and it connects to the other one not only perpendicularly, but also diagonally. L is a measure of the dimensionality which could be any integer varying from 1 (the net spin ladder) to M (the net spin layers). Throughout this work, we use $\mathbf{S}$ to represent spins on the lower layer, and $\mathbf{S}'$ on the upper layer. Open boundary conditions are imposed.

Under certain combination of coupling constants, we show that for general L and M the model could be solved exactly. First, the model have two kinds of ground state, one is a completely dimerized state, and the other one is the ground state of the spin-1 model defined on the single layer. Second, the model exhibits rich excitation phases, depending on coupling constants and dimensionality L. As we shall show below, these properties are quite different from the existing models such as the Majumdar-Ghosh model [1].

The model Hamiltonian is:

$$
\begin{aligned}
H = & 2J_1 \sum_{k,l=1}^{M,L} \mathbf{S}_{k,l} \cdot \mathbf{S'}_{k,l} \\
& + 2J_2 \sum_{k,l=1}^{M-1,L-1} \mathbf{S}_{k,l} \cdot (\mathbf{S}_{k+1,l} + \mathbf{S}_{k,l+1}) + \mathbf{S'}_{k,l} \cdot (\mathbf{S'}_{k+1,l} + \mathbf{S'}_{k,l+1}) \\
& + 2J_3 \sum_{k,l=1}^{M-1,L-1} \mathbf{S'}_{k,l} \cdot (\mathbf{S}_{k+1,l} + \mathbf{S}_{k,l+1}) \\
& + 2J_4 \sum_{k,l=1}^{M-1,L-1} \mathbf{S}_{k,l} \cdot (\mathbf{S'}_{k+1,l} + \mathbf{S'}_{k,l+1}) \ , \qquad (1)
\end{aligned}
$$

with $J_1, J_2, J_3, J_4 \geq 0$, and $|\mathbf{S}| = |\mathbf{S'}| = S = 1/2$. Both J_1 and J_2 favor local antiferromagnetic ordering while J_3 and J_4 represent frustration effects.

For any integers M and L, we found that a complete dimerized state:

$$
\psi_D = [1,1'][2,2'] \cdots [M,M'] \cdots [N,N'], \ N = ML \ , \qquad (2)
$$

where $[i,j]$ denotes the normalized singlet $\frac{1}{\sqrt{2}}(\alpha_i\beta_j - \beta_i\alpha_j)$ with α and β representing the usual up and down single spin eigenfunctions, respectively, is an eigenstate of Eq. (1) when we impose the following constraint:

$$
2J_2 = J_3 + J_4 \ . \qquad (3)
$$

To prove our statement, we first show that this is true for the 4-spin plaque case, $\{\mathbf{S}_{1,1}, \mathbf{S'}_{1',1'}, \mathbf{S}_{2,1'}, \mathbf{S'}_{2',1'}\}$, simplied as $\{\mathbf{S}_1, \mathbf{S'}_{1'}, \mathbf{S}_2, \mathbf{S'}_{2'}\}$, which is indicated in Fig. 1. The model Hamiltonian commutes with total spin S_{tot} so one can use it to characterize eigenstates. In the sub-space of zero z-component magnetization there are six eigenstates and among these six eigenstates there are two singlets which are determined by the following equations:

$$
\begin{aligned}
H\psi_D &= -3J_1\psi_D + \frac{\sqrt{3}}{2}(2J_2 - J_3 - J_4)\psi_2 \qquad (4) \\
H\psi_2 &= \frac{\sqrt{3}}{2}(2J_2 - J_3 - J_4)\psi_D + (J_1 - 2J_2 - J_3 - J_4)\psi_2
\end{aligned}
$$

where

$$
\psi_D = \frac{1}{2}(\alpha_1\beta_{1'} - \beta_1\alpha_{1'})(\alpha_2\beta_{2'} - \beta_2\alpha_{2'}) \qquad (5)
$$

is the completely dimerized state it becomes an eigenstate of H with eigenvalue $-3J_1$ and another singlet state ψ_2 with eigenvalue $E_2 = J_1 - 4J_2$ when Eq. (3) holds.

Also, we obtained other four eigenvalues according to their total spin S_{tot}, among them there is a triplet with eigenvalue:

$$E_3 = -(J_1 + J_2) + \frac{1}{2}(J_3 + J_4) \ . \tag{6}$$

We know that the formation of dimers $[1, 1']$ and $[2, 2']$ is due to antiferromagnetic coupling J_1. Without antiferromagnetic couplings J_3 and J_4, quantum fluctuation due to J_2 will kill both dimers. As long as condition Eq. (3) holds, the effect of J_2 on the dimers will be canceled exactly by J_3 and J_4. This is also true no matter how many plaques we put together and thus ψ_D is the eigenstate of Hamiltonian (1) with eigenvalue $E_D = -\frac{3}{2}MJ_1$.

It is also obvious that the dimerized state ψ_D may not be the ground state for general coupling parameters $\{J_1, J_2, J_3, J_4\}$ due to the fact that the antiferromagnetic couplings J_2, J_3, J_4 which connect one plaque to another also introduce interactions between plaques. Since in the limit of $J_1 \to \infty$, ψ_D must be the ground state, and in the limit of $J_1 \to 0$, ψ_D cannot be the ground state, therefore we expect that there exists a critical value of J_{1c} such that when $J_1 > J_{1c}$ the ground state is completely dimerized.

We should mention that for the case of $L = 1$, the spin net model (we call it net spin ladder) goes back to the Majumdar-Ghosh model [1] when $J_2 = 0.5J_1, J_3 = J_1$, and $J_4 = 0$. Several studies on the generalization of the M-G model, such as the zigzag model [2–7], were carried out before.

To proceed, we study the case of $L = 1$ with coupling constants $J_3 = J_4 = J_2$ in details as an illustration. This special case has been recently studied by several groups [10–15]. We use it as an example to present our approach which leads us to solve the whole class of net spin models.

We can rewrite the Hamiltonian as

$$H = -2MJ_1\frac{3}{4} + J_1 \sum_{k=1}^{M-1} \boldsymbol{\sigma}_k^2 + 2J_2 \sum_{k=1}^{M-1} \boldsymbol{\sigma}_k \cdot \boldsymbol{\sigma}_{k+1} \ , \tag{7}$$

where $\boldsymbol{\sigma}_k = \mathbf{S}_k + \mathbf{S}'_k$. This Hamiltonian describes a chain of M spins with either $|\boldsymbol{\sigma}_k| = 0$(singlet) or 1(triplet).

With this form of H, it is easy to see that ψ_D is an eigenstate of H by using the relation $(\mathbf{S}_k + \mathbf{S}'_k)[k, k'] = 0$, hence

$$\left(J_1 \sum_{k=1}^{M-1} \boldsymbol{\sigma}_k^2 + 2J_2 \sum_{k=1}^{M-1} \boldsymbol{\sigma}_k \cdot \boldsymbol{\sigma}_{k+1} \right) |\psi_D >= 0 \ , \tag{8}$$

and the eigenvalue is $E_D = -\frac{3}{2} M J_1$.

To lower energy, the squared term, $J_1 \boldsymbol{\sigma}_k^2$, favors to be in the $|\boldsymbol{\sigma}_k| = 0$ state, while the exchange term, $J_2 \boldsymbol{\sigma}_k \cdot \boldsymbol{\sigma}_{k+1}$, favors to be in the $|\boldsymbol{\sigma}_k| = 1$ state. If all pairs $\mathbf{S}_k + \mathbf{S}'_k$ are in the $\sigma = 1$ state then the model is equivalent to the spin-1 chain with coupling constant $2J_2$, apart from a constant $\frac{MJ_1}{2}$. One can see from Eq. (7) that the eigenstates of the spin-1 chain could also be the eigenstate of the net spin ladder model. In fact, as J_1 decreases further, the ground state of the net spin ladder model becomes the ground state of the spin-1 chain.

Moreover, we can use this criterion to determine the transition point J_{1c}. When $J_1 = J_{1c}$, $< H >= E_D = -\frac{3}{2} M J_1$, where the expectation value is taken in the ground state. We obtain

$$< J_{1c} \sum_{k=1}^{M-1} \boldsymbol{\sigma}_k^2 + 2J_2 \sum_{k=1}^{M-1} \boldsymbol{\sigma}_k \cdot \boldsymbol{\sigma}_{k+1} >= 0 \ , \tag{9}$$

i.e., $2J_{1c}M$ = ground state energy of M-site spin-1 chain with coupling constant $2J_2$. Using the existing estimates [16], we obtain

$$J_{1c} = 1.4015 J_2 \ . \tag{10}$$

To confirm our analysis, we determine the critical value J_{1c} by using the exact diagonalization technique [17] for several clusters. Our numerical answer is $J_{1c} = 1.402 \pm 0.001$, the same as the above within numerical error.

We next study excitation spectrum of the model. One can create a single magnon simply by breaking a dimer: $\frac{1}{\sqrt{2}}(\alpha_i \beta_j - \beta_i \alpha_j) \to \alpha_i \alpha_j$ (or $\beta_i \beta_j$ or $\frac{1}{\sqrt{2}}(\alpha_i \beta_j + \beta_i \alpha_j)$.) It can be shown that state

$$\psi_m = [1, 1'][2, 2'] \cdots (\uparrow, \uparrow) \cdots [M, M'] \ , \tag{11}$$

is also an eigenstate of the net spin ladder model with total spin $S_{tot} = 1$. The energy gap in this case is exactly $\Delta_{st} = 2J_1$ and the transition is from singlet to triplet. This excitation energy is independent of other antiferromagnetic couplings as long as the condition (3) holds and thus it is possible that there exists states with lower excitation energy.

Analyzing results for the single plaque, we found that when $J_1 < 2J_2$, $E_2 = J_1 - 4J_2$ is lower than $E_3 = -J_1$ of Eq. (6). The former is in the singlet ($S_{tot} = 0$) sector. Interesting enough, this critical value $(J_1/J_2)_c = 2$ is independent of lattice size. This could be easily understood by using the Hamiltonian of Eq. (7). Such excitation corresponds to the situation where two adjunct dimers are broken (so they are in the spin $S = 1$ state) while the rest of dimers remain unbroken, regardless the chain length. The two spin 1 sites form a singlet with energy $-4J_2$ so the excitation energy, which corresponds to the transition from the dimer singlet to another singlet, is $\Delta_{ss} = 4J_1 - 4J_2$. $\Delta_{ss} < \Delta_{st}$ when $J_1 < 2J_2$.

What will happen as one decreases J_1 further? We found that the first excited state remains to be the one we just described for the whole region of $2J_2 > J_1 > J_{1c}$. Moreover, this state is $(M-1)$-fold degenerate. States consisting of longer segment of broken dimers are high in energy.

Figure 2a summarizes our findings. Here gap Δ is defined as the difference between the first excited state energy and the ground state energy, $E(1) - E(0)$. There are three regions, depending on parameter J_2/J_1:

Region I , $J_1 \geq 2J_2$, $\Delta/J_1 = 2$, independent of J_2 and it is singlet to triplet.

Region II , $2J_2 > J_1 > J_{1c}$, $\Delta/J_1 = 4(1-J_2/J_1)$ decreases linearly from 2 to $4(1-J_2/J_{1c}) = 1.1459$ at $J_1 = J_{1c}+$. The excitation is from singlet (dimers) to another singlet. In both regions I and II, the completely dimerized state is the ground state.

However, right at $J_1 = J_{1c}$, the completely dimerized state is degenerate with the ground state of spin-1 chain.

Region III , $J_1 > J_{1c}$, it is the Haldane gap phase. At $J_1 = J_{1c}-$, $\Delta/J_1 = 0.5851$.

We now turn to the double layer case ($L = M$ and $N = LM$). Similarly, we get

$$H = -2NJ_1\frac{3}{4} + J_1\sum_{k=1}^{N}\boldsymbol{\sigma}_k^2 + 2J_2\sum_{<k,l>}^{N}\boldsymbol{\sigma}_k\cdot\boldsymbol{\sigma}_l\ , \tag{12}$$

where $\boldsymbol{\sigma}_k = \mathbf{S}_{k,l} + \mathbf{S}'_{k,l}$ and $< k, l >$ refer to nearest neighbors in two dimensions. Again, when all $|\boldsymbol{\sigma}| = 1$, this is nothing but the two-dimensional antiferromagnetic Heisenberg model with coupling constant $2J_2$, apart from a constant.

With the same approach we had described above, it is easy to see that a complete dimerized state where all $\boldsymbol{\sigma}$ are in singlet state is the eigenstate of the model and it is the ground state when J_1 is sufficiently large. The critical point at which the complete dimerized state becomes the excited state is determined by,

$$J_{1c} = -\frac{J_2}{N}\sum_{<k,l>}^{N}\boldsymbol{\sigma}_k\cdot\boldsymbol{\sigma}_l\ . \tag{13}$$

Using the existing estimates [18], we obtain

$$J_{1c} = 2.3323J_2\ . \tag{14}$$

Two interesting observations are right in hand:

(1) The existence of the critical point is similar to that for the double layer layer antiferromagnetic Heisenberg model without diagonal coupling (J_3 and J_4 set to be zero) terms. There has been a lot of studies on that model, by the spin-wave theory, perturbation theory, bond-operator approach, etc. (Ref. [19] and references therein.) The transition point at which gap vanishes is $J_1/J_2 = 2.54$, close to the value of J_{1c} we got here, although with different model.

(2) We can show that it is still true when $J_1/J_2 \leq 2$, the first excitation is a triplet. Moreover, after $J_1/J_2 \leq 2.3323$, the system is gapless because the existence of long-range-order in the two-dimensional spin-1 Heisenberg model, as shown rigorously long time ago [20,21]. Therefore, there exists no transition from the dimer singlet to another singlet as what we have seen for the net spin ladder case. Note that the numerical accuracy of 2.3323 is unimportant here, as long as the ground state energy per site is lower than $-2J_2$, (which

must be true because $-2J_2$ just corresponds to the Neel state!), our assertion holds. We plot the excitation gap as function of J_2/J_1 in Fig. 2b.

What will happen for cases of $1 < L < \infty$? We have studied two cases, $L = 2$ and $L = 3$. For $L = 2$, the critical value J_{1c} is determined by the corresponding spin-1 model defined on the $2 \times M$ lattice. Table I. lists the ground state energy per site as well as per bond. Total number of lattice sites is $N = 2 \times M$ and total number of bonds is $N_b = 3 \times M - 2$ when open boundary is used.

It is clear that, in the limit of $N \to \infty$, we have

$$E/NJ_2 = (E/N_b)(N_b/N) = (3/2)(E/N_b) \tag{15}$$
$$> (1.5) * (-1.3) = -1.95 > -2.0.$$

Thus, $J_{1c} < 2J_2$ and the excitation spectrum for the case of $L = 2$ is similar to that of $L = 1$.

Similarly, we list the ground state energy per site as well as per bond in Table II for the case of $L = 3$.

Because we do not have enough data due to lack of computer power, we cannot confidently establish a lower bound for the ground state energy in the thermodynamics limit. Although a second order perturbation theory calculation gives

$$E/NJ_2 = -\frac{617}{315} > \frac{630}{315} = -2 \ , \tag{16}$$

it is too close to be definitive. On the other hand, the second order perturbation theory calculation for the $L = 2$ case gives

$$E/NJ_2 = -\frac{9}{5} > -2 \ , \tag{17}$$

which is more definitive.

Therefore, we cannot rule out a possibility of dimensional crossover from 1-D to 2-D occurs at $L = 3$. It is also equal probable that $J_{1c} < 2J_2$ but the difference between J_{1c} and $2J_2$ becomes exponentially small when L increases from 3.

For other combinations of couplings, one can only determine the critical points and eigenvalues of the model numerically. However, qualitative behaviors should be the same as what we have shown here. Note that the energy gap $2J_1$ is quite large (critical values of J_2 are smaller than J_1) so the phase diagram should be similar to Fig. 2. Also we note that one obtains a critical value of $J_1/J_2 = 2.54$ when $J_3 = J_4 = 0$ is very close to that when $J_3 = J_4 = J_2 = (1/2.33)J_1$. This shows that our results are insensitive to the values of J_3 and J_4. Essential physics is determined by the two couplings: J_2 and J_1.

In summary, we have studied a class of net spin models, defined by the Hamiltonian Eq. (1), and controlled by three antiferromagnetic couplings: J_2/J_1, J_3/J_1, J_4/J_1, and dimensionality L. When $2J_2 = J_3 + J_4$, the completely dimerized state ψ_D is an eigenstate of these models and it is also the ground state if J_1 is sufficiently large. To fully understand the model, we have studied the case of $J_2 = J_3 = J_4$ extensively and obtained phase diagrams for both 1-D(ladder, $L = 1$) and 2-D(double layer, $L = M$) cases. For the ladder case at a particular point in the parameter space: $J_2 = \frac{1}{2}J_1$, $J_3 = J_1$, and $J_4 = 0$ this model returns to the Majumdar-Ghosh model [1]. But its behavior is quite different from that of the Majumdar-Ghosh model. We also show qualitative different behavior between the ladder and the double layer cases. Moreover, we have studied the cases of $L = 2$ and $L = 3$ and discussed the possibility of crossover from 1-D to 2-D. In addition, we made connection with other studies of double layer system.

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FIGURES

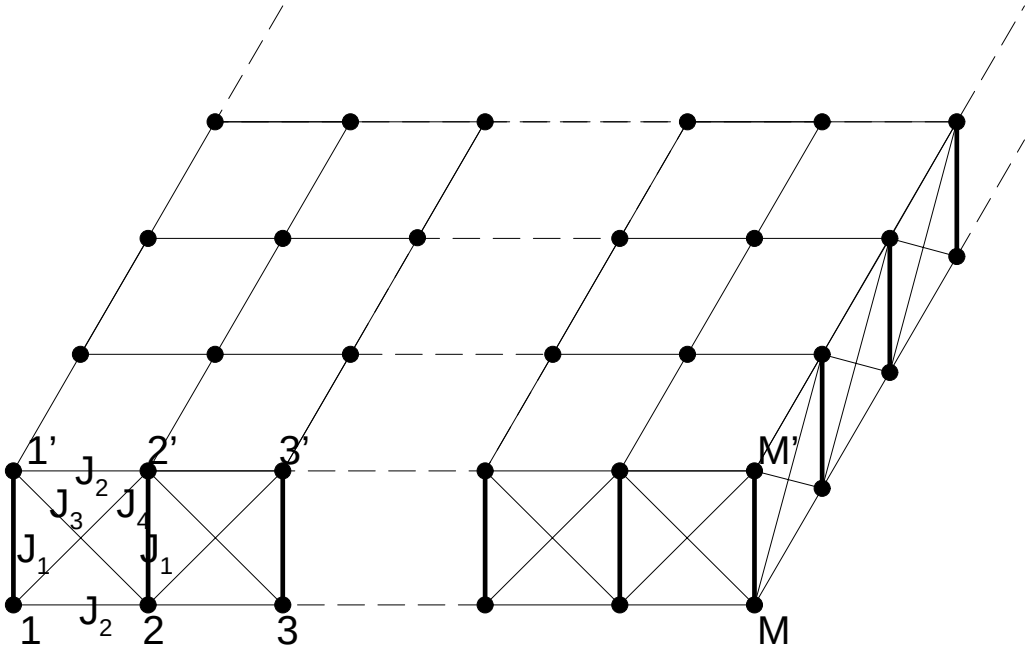

FIG. 1. The net spin layers of $2ML$ spins, where thick solid lines represent singlet dimers.

Fig. 2a

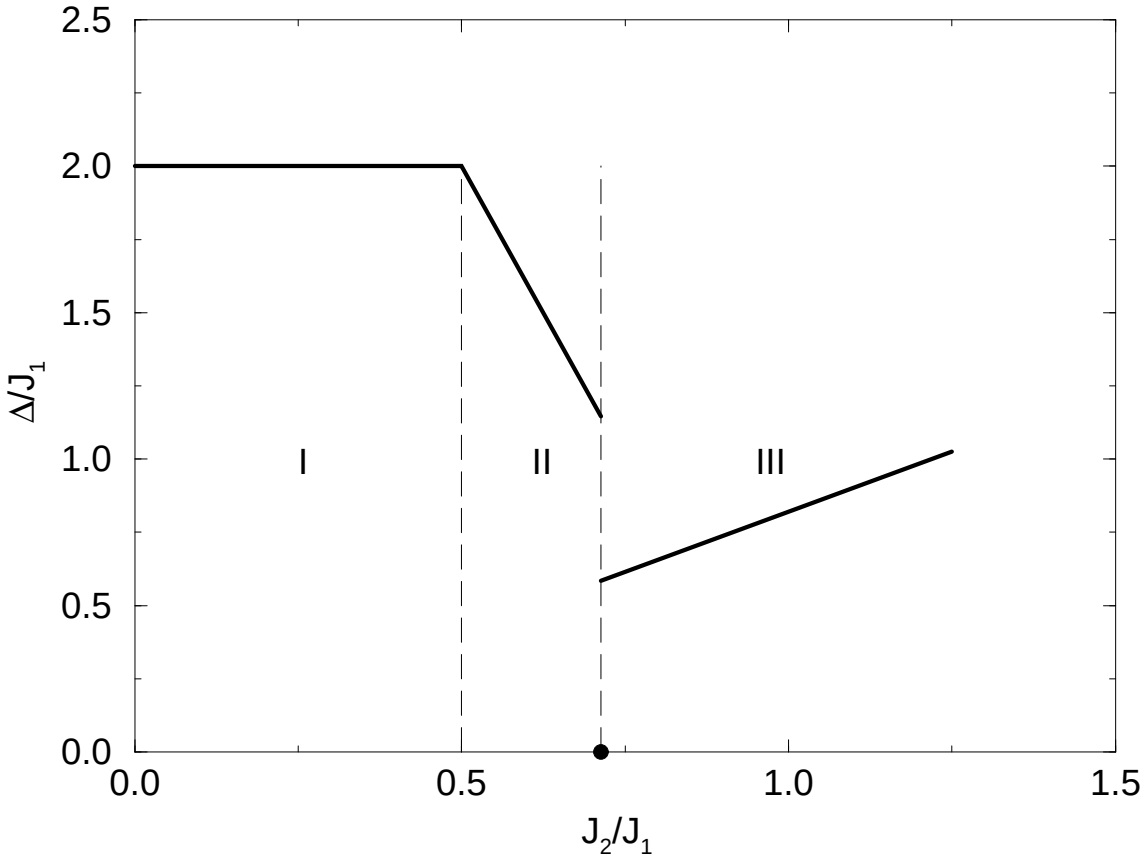

Fig. 2b

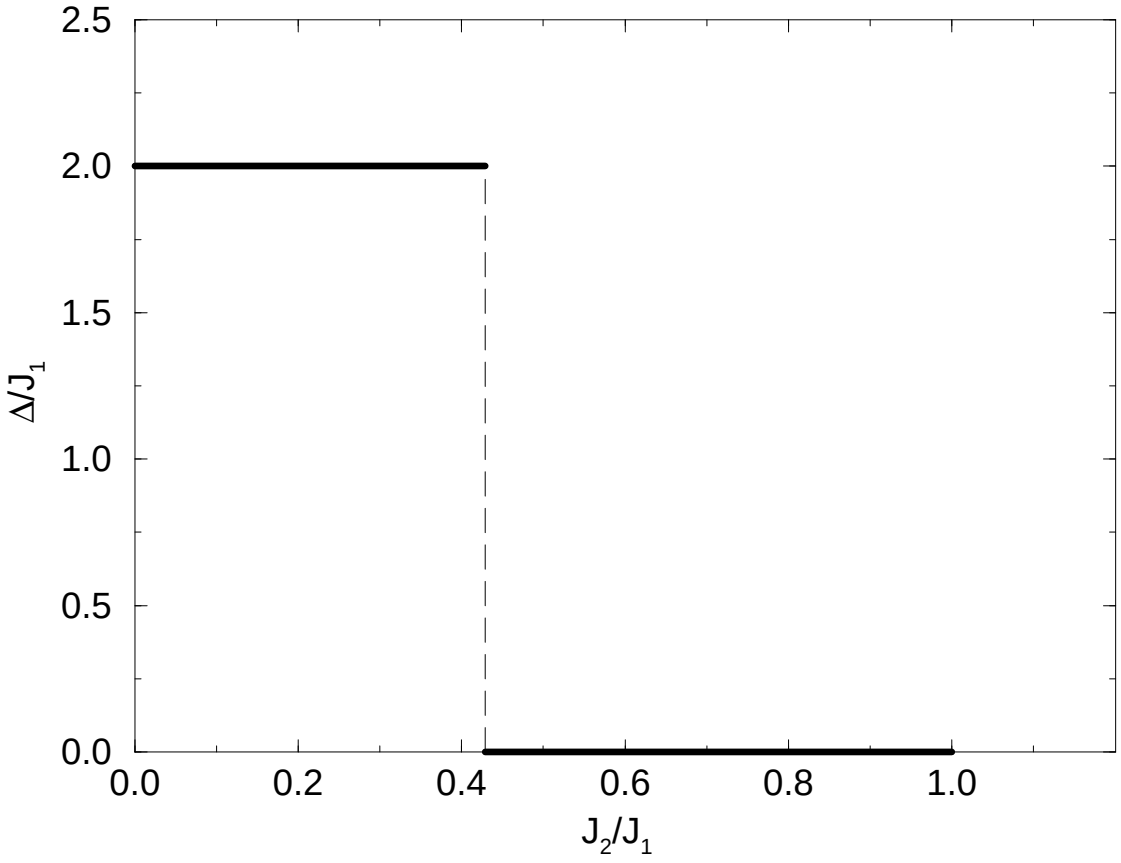

FIG. 2. Excitation gap as function of coupling parameters for the net spin ladder (a), and double layer (b) models.

Table I

Lattice	$E(0)/N$	$E(0)/N_b$
2×2	-1.50000000	-1.50000000
2×3	-1.61633441	-1.38542949
2×4	-1.68229677	-1.34583741
2×5	-1.72097660	-1.32382816
2×6	-1.74706131	-1.31029598
2×7	-1.76571007	-1.30104952
2×8	-1.77973127	-1.29435001

Table II

Lattice	$E(0)/N$	$E(0)/N_b$
3×2	-1.61633441	-1.38542949
3×3	-1.71359964	-1.28519973
3×4	-1.80819446	-1.27637256
3×5	-1.83887667	-1.25377955